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Supporting information

Electrochemical Storage Mechanism in oxy-Hydroxyfluorinated Anatase for Sodium-ion Batteries

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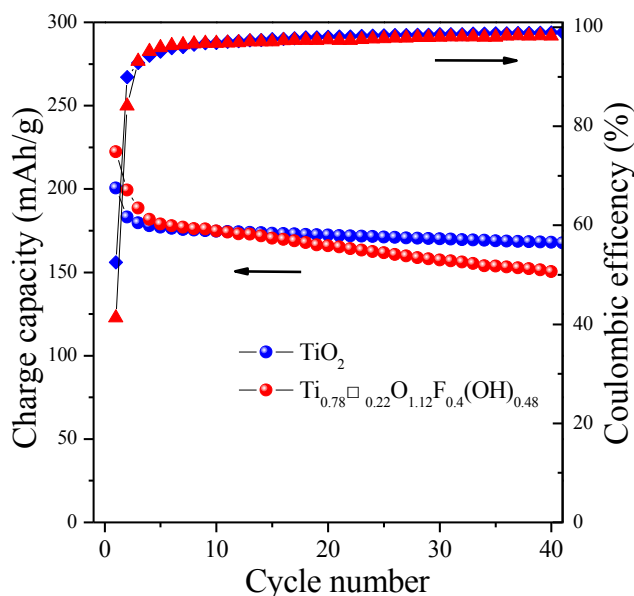


Figure S1. Cycling behavior of $\text{Ti}_{0.78}\square_{0.22}\text{O}_{1.12}\text{F}_{0.4}(\text{OH})_{0.48}$ vs. TiO_2 . The cell was cycled between 0 – 2 V at a current density of 25 mA/g.

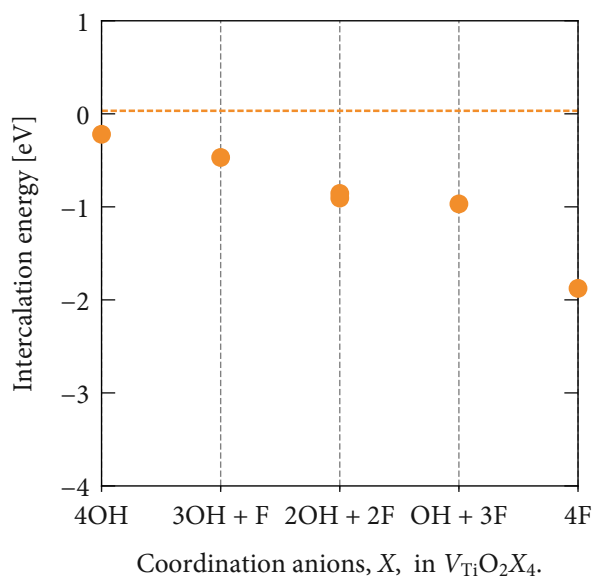


Figure S2. Intercalation energy of lithium in a $Ti_{35}O_{68}X_4$ supercell with $X = F^-, OH^-$. The horizontal dashed line shows the intercalation energy for lithium in stoichiometric anatase TiO_2 . Source: The data set and code to generate this figure, and the figure file, are available under the MIT licence as part of ¹.

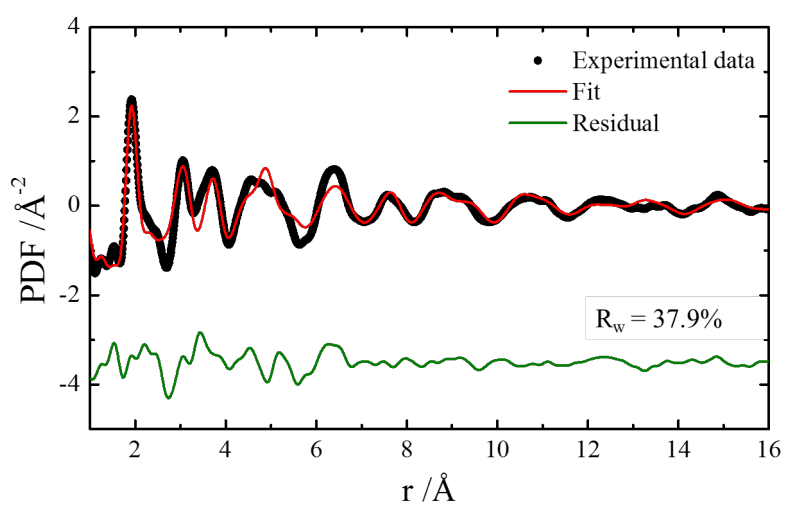


Figure S3. PDF refinement of the electrode charged to 2.0 V using TiO_2 anatase and O3-type Na_xTiO_2 (space group: R-3m) model.

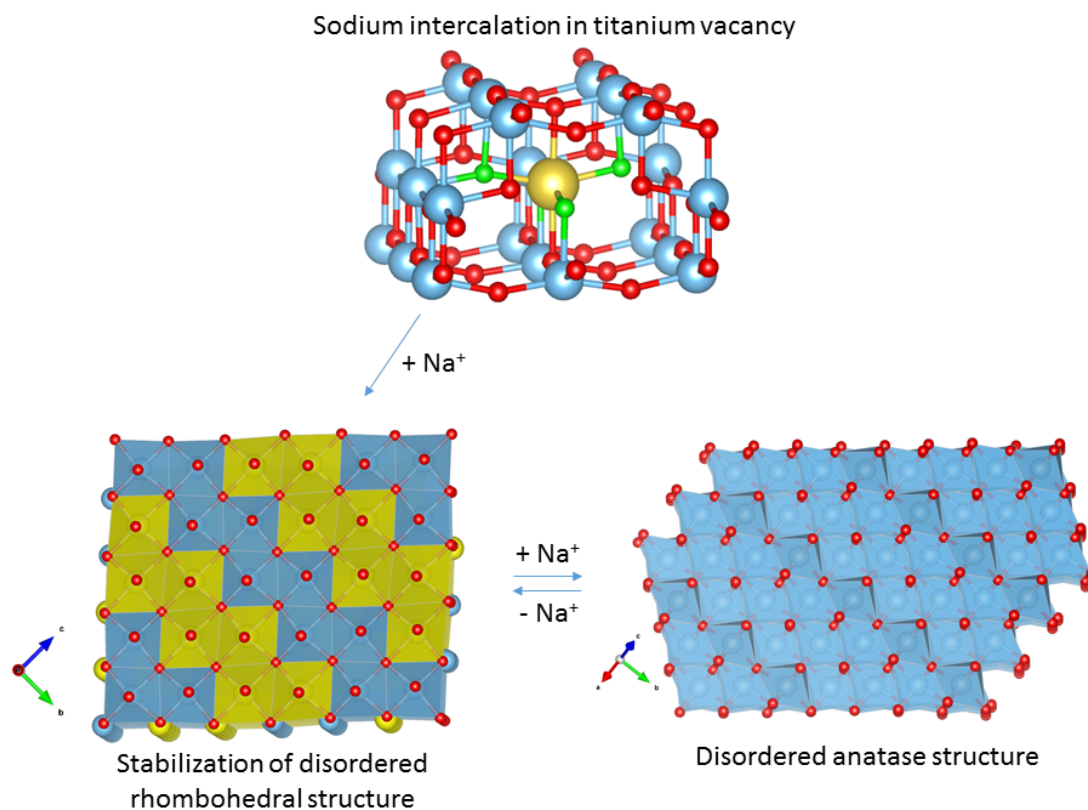


Figure S4. Structural representation of the sodium storage mechanism occurring in defective anatase.

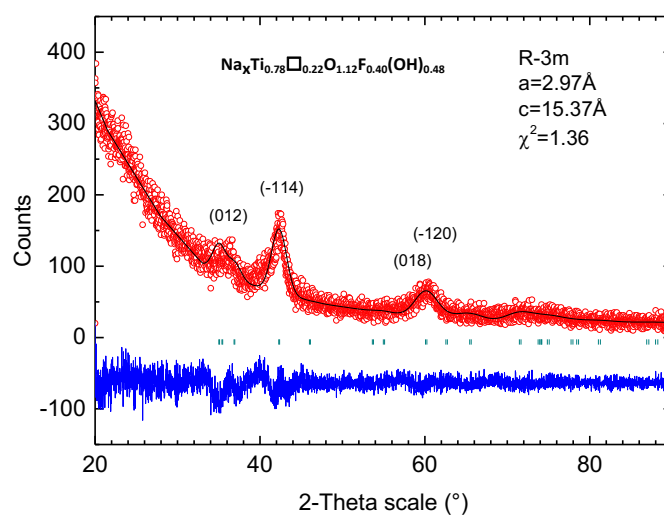


Figure S5. Le Bail profile refinement of the x-ray diffraction powder pattern of the reduced $\text{Na}_x\text{Ti}_{0.78}\square_{0.22}\text{O}_{1.12}\text{F}_{0.40}(\text{OH})_{0.48}$ obtained by chemical sodiation.

Reference

- 1 B. J. Morgan, DFT Data Analysis: Intercalation of X=(Li, Na, Mg, Ca, Al) into (F/OH)-substituted anatase TiO_2 . Zenodo 2017, <http://doi.org/10.5281/zenodo.1181872>.